Saurabh Singh

Department of Materials Science and Engineering
Pennsylvania State University
Steidle Building, University Park,
PA,16802 United States
TEL +1 (814) 321-4910
E-mail sbs6760@psu.edu saurabhsingh950@gmail.com

Research Experience

- **Postdoctoral Fellow**, January 2022 – present, Department of Materials Science and Engineering, The Pennsylvania State University, Steidle Building, University Park, PA, 16802 United States.
- **Commissioned Scientist**, 1st November 2021 – December 2021, Energy Materials Laboratory, Toyota Technological Institute, Nagoya Japan.
- **Postdoctoral Fellow**, November 2018 – October 2021, Energy Materials Laboratory, Toyota Technological Institute, Nagoya Japan.
- **Institute Postdoctoral Fellow**, July 2018 - October 2018, Indian Institute of Technology Bombay, Mumbai, India.
- **Visiting researcher**, May-June 2018, Energy Materials Laboratory, Toyota Technological Institute, Nagoya Japan.
- **Research Fellow,** July 2010 – December 2012, UGC Department of Atomic Energy, Consortium for Scientific Research, Indore, Madhya Pradesh, India.

Education and degrees

- **Doctor in Philosophy (Ph.D)** in Condensed Matter Physics (Feb 2013 – May 2018), School of Engineering, Indian Institute of Technology Mandi, Himachal Pradesh, India.
  Dissertation title: "*Thermoelectric Properties of Oxides Materials in High Temperature Region*".
  Supervisor: Dr. Sudhir K. Pandey.
- **Master in Philosophy (M.Phil)** in Physics (2010 - 2011), School of Physics, Devi Ahilya Vishwavidyalaya, Indore, India.
- **Master in Science (M.Sc.)** in Physics (2007 - 2009), University of Mumbai, Mumbai, India.
- **Bachelor in Science (B.Sc.)** in Physics (2004 – 2009), Thakur College of Science and Commerce, Mumbai, India.

Distinctions, scholarships and awards

- Best **oral** presentation award at IIT Mandi **Research Fair** in 2017.
- Best **oral** presentation award (NSMCU-2012), Amity School of Science & Technology Delhi, India.
- Graduate Aptitude Test in Engineering (**GATE**) 2012.
- Joint Entrance Screening Test (**JEST**) 2010.
- National Graduate Physics Examination (**NGPE**) award by Indian Association of Physics Teachers in 2006.
- B.Sc, MSc, M.Phil with **throughout distinctions**.
- International **travel award** for research presentation **International Conference on**

Thermoelectrics 2017, in **California Institute of Technology**, Pasadena, **USA**, supported from SERB, Department Science and Technology India.

- International **travel award** for research presentation **IUMRS-ICAM 2017**, The 15th International Conference on Advanced Materials, 27th August - 1st September 2017, Yoshida Campus **Kyoto University, Kyoto, Japan**, supported from SERB, Department Science and Technology, India.

Research Interest

- Condensed Matter Physics and Materials Science

Research Keywords

- Crystal Structure, Electronic Structure, Transport properties, Thermoelectrics, Thermal Diodes, Thermal Rectifiers, Thermomagnetics, Magnetocaloric, Multiferroics

Research Materials

- Oxides, Chalcogenides, Sillicon-Germanium alloys, Heusler alloys, Skutterudites, Heavy Fermions

Computational and Experimental Skills

- **Crystal Structure optimizations** and **electronic structure** calculations using **DFT** and **DFT+*U*** methods implemented in **VASP**, **Wien2K**, **Akai KKR-CPA**, **SPR-KKR**, **Quantum Espresso**, **ELK-LAPW**, **STATE** codes. **Phonon dispersion**, and **thermal transport properties** using **phonopy** and **phono3py** codes.
- **Transport coefficient** calculations using "*Semi classic Boltzmann transport theory*" implemented in **BoltzTraP** code.
- **Heat flow modeling** for **thermal management** using **COMSOL multiphysics.**
- **Hand on experience** of **computational** work using DFT codes installed in **cluster as common platform** in **IIT Mandi** India, MEMS **IIT Bombay** India, University Cluster **Osaka University** Japan, **Super-computer** in **Institute of Molecular Science** Okazaki Japan.
- In house development of **Seebeck coefficient** and **Electrical Resistivity** measurement systems for **bulk** and **thin film** samples in **80-1100 K** temperature range.
- Development of automatic system for output power measurement of **Thermoelectric device**.
- **Programming** using **LabVIEW** interfacing code for data acquisition and hardware control.
- Fabrication of **prototype** and **π-type** Thermoelectric **Devices**.
- **Sample preparation** of oxide, Chalcogenides, Si-Ge alloys, Heusler alloys by Chemical Synthesis, Solid State Reaction route, Melting Method, Spark Plasma Sintering, Arc Melting, Ball Milling, RF Sputtering, Molecular Beam Epitaxy.
- *Rietveld refinement* of X-ray diffraction pattern using FullProf Suite, thermal stability using DSC, TGA-DTA, **Physical property measurements** using PPMS (9 Tesla) Quantum Design, chemical composition analysis using SEM-EDX, EPMA.
- **Synchrotron measurements** facility used in **BL05 X-ray diffraction** at **Aichi Synchrotron Centre** Nagoya, **BL09 HAXPES and BL02B X-ray diffraction** at **SPRING8** Hyogo, Japan.

- **Neutron diffraction measurements** used in **BL08 SuperHRPD Japan Proton Accelerator Research Complex (JPARC)**, Ibaraki, Japan.

Detailed Descriptions of the Research Work

Current Research:

Since January 2022 at Penn State University, actively working on **Gd (Si,Ge) based magnetic phase transition materials** and **tailoring the thermomagnetic properties** by combine use of experiment and DFT calculations. The main goal of the research is to **find the materials** which show **high magnetic properties** with **ferro-paramagnetic transition near room temperature** together with **large thermal conductivity** for efficient energy harvest.

(1) Research history

In IIT Mandi, India (Ph.D. student, 2013-2018)

Focused on **thermoelectric materials** in making Seebeck coefficients and electrical resistivity measurement systems and investigated the effect of **electronic structure on electron transport properties** of oxides by combined use of **experiment tools** and **density functional theory calculations**. Investigated the high-temperature (300-600 K) thermoelectric behavior of oxides including ZnV_2O_4, $LaCo_{1-x}Ba_xO_3$ (x = 0, 0.18, 0.25), $(La_{0.7}Sr_{0.3}MnO_3)_{1-x}(NiO)_x$ (x = 0, 0.5) systems, to find its practical applicability for thermoelectric applications [*see publications no.* **1-9**].

In Toyota Technological Institute, Japan (Postdoc, 2018-2021)

The objective of research in Toyota Technological Institute was mainly focused on the **Silver chalcogenides (Ag_2X, X = S, Se, Te)**, which shows very low thermal conductivity (0.5 - 1 Watt m^{-1} K^{-1}) and moderate Seebeck coefficients (~ -100 μV/K) about room temperature. Ag_2S possess excellent flexibility with very large Seebeck coefficients due to insulating nature, but due to very high electrical resistivity (~10^6 mohm cm), prevent us to use it as thermoelectric materials near 300 K. By selenium substitutions at sulfur site i.e. ($Ag_2S_{1-x}Se_x$, $0 \leq x \leq 1$), **we have successfully decrease the electrical resistivity** (increase electrical conductivity**) by 10^6 order**, together with maintaining low thermal conductivity (less than unity), and moderate Seebeck coefficients, which results into the **enhancement of the thermoelectric property** of this material leading to the thermoelectric ***figure of merit*** **about unity** [**10**]. Very interestingly, we noticed that high performance temperature shifted close to room temperature, which is very good signature for the practical applications. Importantly, with Se substitutions Ag_2S system up to the composition $Ag_2S_{0.45}Se_{0.55}$ possess very good flexibility, when rolled it, and allow it in self-standing condition without any external substrate or flexible support.

(2) Additional Collaborative Research Work (Bulk, thin-films, single crystals)

With **constructive modifications of electronic structure** near chemical potential in Si-Ge alloys, i.e. by formation of impurity peak in electronic density of states near band edge, and **nanostructuring** the large values of *figure of merit* in both *p* and *n*-type materials are effectively achieved for **thermoelectric applications** in high temperature region [**11** - **13**].

The understanding of transport properties of **wide band gap materials** has always been challenging both experimentally and computationally. To overcome the constrain of fundamental issue typically faced in characterization of Seebeck coefficient of insulating materials while using the commercial measurement setup, a simple and low cost of **measurement system** is developed [**14**]. Furthermore, the electronic structure calculations using GGA and meta-GGA exchange correlation functional, the transport properties mainly focused from thermoelectric applications, in 80 – 650 K temperature range, point of view were successfully investigated on **single crystal GaN** and β-Ga_2O_3 materials [**15-16**]. The role of **anisotropic electronic structure** led to the enhancement of thermoelectric properties of α-$YAlB_4$ **singe crystal** in cryogenic temperature regime is explored [**17**].

Silver and **copper chalcogenide** (Ag_2S, Ag_2Se, Ag_2Te, Cu_2S, Cu_2Se) materials go through the structural and electronic phase transition in 300- 500 K range, as a result an **abrupt change in electronic and heat transport properties** is observed. We systematically investigated the **colossal transport properties** across the phase transition, and successfully identified the conditions which provides potential applicability of these materials for **thermoelectric**, **thermal diode**, **thermal rectifiers** applications [**18-24**].

To achieve the large thermoelectric performance lower magnitude of thermal conductivity with optimized carrier concentration provided by the suitable electronic structure is require. Generally, most of the oxides and Heusler alloys possess high thermal conductivity due to large contribution from the lattice part. We have successfully suppressed the lattice thermal conductivity by incorporation of reduced graphene oxides in Al doped ZnO material and achieved large thermoelectric performance [**25**]. The combined effect of **lattice softening** and **band convergence** lead to **large thermoelectric performance** in mid-temperature range in **co-doped SnTe** [**26**]. Using the **electronic** and **phonon dispersion calculations**, we studied the role of light and heavy mass elements substitutions in tuning the **electronic transport** coefficients and the **thermal conductivity** of heusler alloys $Fe_{2-x}Mn_xCrAl$ **(0<*x*<1) and** $ZrIr_{1-x}CoxSb$ **(0<x<1)** systems, and it is **experimentally verified** [**27-29**].

Several oxides systems (nanomaterials, bulk, and thin films) have also been investigated including structural, electrical, magnetic, dielectric, photocatalytic, and thermoelectric properties. For its thermoelectric applications, **oxides** and **skutterudite thin films** are investigated for potential uses in high temperature region [**30**- **39**].

Academic and Scientific Experience

- **Lab setup** from the scratch by in-house development of measurement systems which outcome led to the Ph.D. degree.
- **Establishment of experimental facilities** in Physics Laboratory (PH 515P) for Integrated PhD (i-PhD) course experiment, Lab-teaching assistant **IIT Mandi**, Aug-Dec. 2016.
- **Mentoring research projects** of I-Phd (Materials Science) and M.Sc. (Physics) **IIT Mandi**.
- **Research academic Secretary** year 2014 - 2015 **IIT Mandi**, India. A representative on behalf of MS and PhD scholar for improvement and betterment of researchers.
- **Invited Chairperson** for handling the oral talks (**Japan session**) in **Virtual Conference on Thermoelectrics** 2021 (at Zoom platform).

Book Chapter Contribution

- **Recent Advances in Energy Harvesting from Waste Heat using Emergent Thermoelectric Materials**", ***Saurabh Singh,*** *Keisuke Hirata, Sudhir K. Pandey, Tsunehiro Takeuchi,* book entitled "***Emerging Materials: Design, Characterization and Applications***" pp 155- 184, Springer Nature Singapore Pte Ltd. 2022.

List of Publications (in Peer reviewed journals)

1. Investigation of the Thermoelectric Properties of ZnV_2O_4 Compound at High Temperatures, ***Saurabh Singh***, *R. K. Maurya and Sudhir K. Pandey,* **J. Phys. D: Appl. Phys. 49**, 425601 (2016).
2. The importance of temperature dependent energy gap in the understanding of high temperature thermoelectric properties, ***Saurabh Singh*** *and Sudhir K. Pandey*, **Mat Res Express 3**, 105501 (2016).
3. An important role of temperature dependent scattering time in understanding the high temperature thermoelectric behavior of strongly correlated system: $La_{0.75}Ba_{0.25}CoO_3$, ***Saurabh Singh***, *Devendra Kumar and Sudhir K. Pandey*, **J. Phys.: Condens. Matter 29**, 105601 (2017).
4. Experimental and theoretical investigations of thermoelectric properties of $La_{0.82}Ba_{0.18}CoO_3$ compound in high temperature region, ***Saurabh Singh***, *Devendra Kumar and Sudhir K. Pandey,* **Phys. Lett. A 381**, 3101 (2017).
5. Understanding the Thermoelectric Properties of $LaCoO_3$ Compound, ***Saurabh Singh*** *and Sudhir K. Pandey*, **Philos. Mag. 97**, 451 (2017).
6. Fabrication of a simple apparatus for the Seebeck coefficient measurement in high temperature region, ***Saurabh Singh*** *and Sudhir K. Pandey*, **Measurement 102**, 26 (2017).
7. Fabrication of Simple Apparatus for Resistivity Measurement in High Temperature Range 300-620 K, ***Saurabh Singh*** *and Sudhir K. Pandey* **IEEE Transactions on Instrumentation and Measurement *67*,** *no. 9: 2169-2176 (2018).*
8. Effect of nanostructure on thermoelectric properties of $La_{0.7}Sr_{0.3}MnO_3$ in 300–600 K temperature range, ***Saurabh Singh****, *Simant Kumar Srivastav, Ashutosh Patel, Ratnamala Chatterjee, and Sudhir K. Pandey*, **Mat Res Express 5**, 055026 (2018).
9. Enhancement in Thermoelectric Properties of *n*-type $(La_{0.7}Sr_{0.3}MnO_3)_{0.5}$ $(NiO)_{0.5}$: Composite and Nano-structure Effect*,* ***Saurabh Singh****, Simant Kumar Srivastav, Ashutosh Patel, Ashish Kumar Ratnamala Chatterjee, Tsunehiro Takeuchi, and Sudhir K. Pandey* **J. Phys. D: Appl. Phys. 55,** 065503 (2022).
10. Investigation of Thermoelectric Properties of $Ag_2S_xSe_{1-x}$ (x= 0.0, 0.2 and 0.4), ***Saurabh Singh***, *Keisuke Hirata, Dogyun Byeon, Takuya Matsunaga, Omprakash Muthusamy, Swapnil Ghodke, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, and Tsunehiro Takeuchi*, **J. Electron. Mater. 49,** 2846–2854 (2020).
11. Au and B co-doped *p*-type Si-Ge nanocomposites possessing ZT= 1.63 synthesized by ball milling and low-temperature sintering, *Muthusamy Omprakash, Kévin Delime-Codrin, Swapnil Ghodke,* ***Saurabh Singh****, Shunsuke Nishino, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, Santhanakrishnan Harish, Masaru Shimomura and Tsunehiro Takeuchi*, **Japanese Journal of Applied Physics 58**, no. 12 : 125501 (2019).
12. Enhancement of the Thermoelectric Performance of Si-Ge Nanocomposites Containing a Small Amount of Au and Optimization of Boron Doping, *Omprakash Muthusamy, Swapnil Ghodke,* ***Saurabh Singh****, Kévin Delime-Codrin, Shunsuke Nishino, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, Santhanakrishnan Harish, Masaru Shimomura & Tsunehiro Takeuchi*, **J. Electron. Mater. 49**, 2813–2824 (2020).

13. Synergetic Enhancement of the Power Factor and Suppression of Lattice Thermal Conductivity via Electronic Structure Modification and Nanostructuring on a Ni- and B-Codoped *p*-Type Si–Ge Alloy for Thermoelectric Application, *Muthusamy Omprakash, **Saurabh Singh**, Keisuke Hirata, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, Santhanakrishnan Harish, Masaru Shimomura, Tsunehiro Takeuchi*, **ACS Appl. Electron. Mater. 3,** 5621-5631, (2021).

14. Apparatus for Seebeck coefficient measurement of wire, thin film, and bulk materials in the wide temperature range (80–650 K), *Ashish Kumar, Ashutosh Patel, **Saurabh Singh** Asokan Kandasami, Dinakar Kanjilal*, **Review of Scientific Instruments**, **90**, 104901 (2019).

15. Role of Carrier Concentration in Thermoelectric Properties of GaN: An Experimental and Theoretical Investigation", *Ashish Kumar, **Saurabh Singh**, Ashutosh Patel, Asokan Kandasami, and Dinakar Kanjila*l, **Phys. Chem. Chem. Phys., 23**, 1601-1609 (2021).

16. Wide range temperature-dependent (80-630 K) study of Hall effect and the Seebeck coefficient of *β*-Ga_2O_3 single crystals", *Ashish Kumar, **Saurabh Singh**, Bhera Ram Tak, Ashutosh Patel, K. Asokan, D. Kanjilal* **Appl. Phys. Lett. 118**, 062102 (2021).

17. Simultaneous enhancement of thermopower and electrical conductivity in the quasi-one-dimensional single crystal *α*-$YbAlB_4$, *Kentaro Kuga, Masaharu Matsunami, **Saurabh Singh**, Satoru Nakatsuji , and Tsunehiro Takeuchi*, **Applied Physics Letters 119**, 223905 (2021).

18. High-Performance Solid-State Thermal Diode Consisting of Ag_2(S, Se, Te), *Hirata, Keisuke, Takuya Matsunaga, **Saurabh Singh**, Masaharu Matsunami, and Tsunehiro Takeuchi*, **J. Electron. Mater. 49,** 2895–2901 (2020).

19. Development of High-Performance Solid-State Thermal Diodes using Unusual Behavior of Thermal Conductivity Observed for Ag_2Ch (*Ch* = S, Se, Te), *Keisuke Hirata, Takuya Matsunaga, **Saurabh Singh**, Masaharu Matsunami and Tsunehiro Takeuchi*, **Mater. Trans. 61**, No. 12 pp. 2402-2406 (2020).

20. A Field Effect Heat Flow Switching Device, Takuya Matsunaga, Keisuke Hirata, **Saurabh Singh**, Masaharu Matsunami, Tsunehiro Takeuchi, **Mater. Trans. 62**, 16-19 (2021).

21. Long-Term Stability of the Colossal Seebeck Effect in Metallic Cu_2Se, *Byeon Dogyun, Robert Sobota, **Saurabh Singh**, Swapnil Ghodke, Seongho Choi, Naoto Kubo, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, and Tsunehiro Takeuchi*, **J. Electron. Mater. 49,** 2855–2861 (2020).

22. Dynamical variation of carrier concentration and colossal Seebeck effect in Cu_2S low-temperature phase, *Byeon Dogyun, Robert Sobota, Keisuke Hirata, **Saurabh Singh**, Seongho Choi, Masahiro Adachi, Yoshiyuki Yamamoto, Masaharu Matsunami, and Tsunehiro Takeuchi.* **Journal of Alloys and Compounds 826**, 154155 (2020).

23. Mixed-phase effect of high Seebeck coefficient and low electrical resistivity in Ag_2S", *Gareoung Kim, Dogyun Byeon, Saurabh Singh, Hirata Keisuke, Seoungho Choi, Matsunami Masaharu, Takeuchi Tsunehiro*, **J. Phys. D: Appl. Phys. 54**, 115503 (2021).

24. Capacitor Type Thin-Film Heat Flow Switching Device, *Keisuke Hirata, Takuya Matsunaga, **Saurabh Singh**, Masaharu Matsunami, and Tsunehiro Takeuchi*, **Japanese Journal of Applied Physics 60,** 124004 (2021).

25. Selective Enhancement in Phonon Scattering leads to High Thermoelectric Figure of Merit in Graphene Oxide encapsulated ZnO nanocomposites" *Soumya Biswas, **Saurabh Singh**, Shubham Singh, Shashwata Chattopadhyay, K. K. H. De Silva, M. Yoshimura, J. Mitra, Vinayak Kamble*, **ACS Applied Material & Interfaces 13**, 23771- 23786 (2021).

26. Physical insights on the lattice softening driven mid-temperature range thermoelectrics of Ti/Zr-inserted SnTe – an outlook beyond the horizons of conventional phonon scattering and excavation of

Heikes, *Ahmad Rifqi Muchtar, Bhuvanesh Srinivasan, Sylvain Le Tonquesse,* ***Saurabh Singh****, Nugroho Soelami, Brian Yuliarto, David Berthebaud, Takao Mori,* **Adv. Energy Mater. 11,** 2101122 (2021).

27. Anomalous dependence of thermoelectric parameters on carrier concentration in Mn-substituted Fe_2CrAl Heusler alloy, *Kavita Yadav,* ***Saurabh Singh****, Omprakash Muthuswamy, Tsunehiro Takeuchi, and K. Mukherjee,* **Philosophical Magazine 102**, 4, 357 (2022).

28. Optical phonon modes assisted thermal conductivity in *p*-type ZrIrSb Half-Heusler alloy: A combined experimental and computational study, *Kavita Yadav,* ***Saurabh Singh****, Tsunehiro Takeuchi, and K. Mukherjee.* **J. Phys. D: Appl. Phys**. **54**, 495303 (2021).

29. Unravelling the phonon scattering mechanism in Half-Heusler alloys $ZrCo_{1-x}Ir_xSb$ (x = 0, 0.1, and 0.25), *Kavita Yadav,* ***Saurabh Singh****, Omprakash Muthuswamy, Tsunehiro Takeuchi, and K. Mukherjee,* **Journal of Physics: Condensed Matter 34,** 035702 (2022).

30. Oxygen Deficient Lanthanum Doped Cerium Oxide Nanoparticles for Potential Applications in Spintronics and Photocatalysis", *Surjeet Chahal,* ***Saurabh Singh****, Ashok Kumar, Parmod Kumar* **Vacuum 177,** 109395 (2020).

31. Influence of Zn (II) on the structure, magnetic and dielectric dynamics of nano-$LaFeO_3$, *Lakshmana T. Rao, M. K. Pradhan,* ***Saurabh Singh****, and S. Dash,* **J Mater Sci: Mater Electron 31,** 4542–4553 (2020).

32. Understanding the role of Ni ions on Photocatalytic activity and Dielectric properties of Hematite Nanostructures: Experimental and DFT approach, *Suman, Surjeet Chahal,* ***Saurabh Singh****, Pratibha Goel, Ashok Kumar, Ompal Singh, and Parmod Kumar*, **Journal of Physics and Chemistry of Solids 156,** 110118 (2021).

33. Phase Transformation and Structural Evolution in Iron Oxide Nanostructures, *Suman, Seema Devi, Vikas Sharma, Surjeet Chahal, Pratibha Goel,* ***Saurabh Singh****, Ashok Kumar, and Parmod Kumar*, **Materials Science & Engineering: B 272,** 115329 (2021).

34. Photocatalytic Activity of α-Fe_2O_3@CeO_2 and CeO_2@α-Fe_2O_3 core-shell nanospheres for degradation of Rose Bengal dye, *Suman,* ***Saurabh Singh****, Ankita, Ashok Kumar, Navish Kataria, Sandeep Kumar, Parmod Kumar,* **Journal of Environmental Chemical Engineering 9,** 106266 (2021).

35. Effect of implantation of Nitrogen ions into VO_2 thin films, Manish Kumar, Saurabh Singh, Weon Cheol Lim, Keun Hwa Chae and Hyun Hwi Lee, **Materials Letters 310,** 131438 (2022).

36. An efficient and unique method for the growth of spindle shaped Mg-doped cerium oxide composed of nanorods for photodegradation of *p*-Nitrophenol Surjeet Chahal, Lakshita Phor, **Saurabh Singh**, Amanvir Singh, Jaideep Malik, Pratibha Goel, Ashok Kumar, Ankita, Parmod Kumar, **Ceramics International** (2022) [Accepted]

37. Investigation on the power factor of skutterudite $Sm_y(Fe_xNi_{1-x})_4Sb_{12}$ thin films: Effects of deposition and annealing temperature*, Giovanna Latronico, Paolo Mele, Cristina Artini, Pietro Manfrinetti, Sian Wei Pan, Yukihiro Kawamura, Chihiro Sekine,* ***Saurabh Singh****, Tsunehiro Takeuchi, Takahiro Baba, Cédric Bourgès and Takao Mori,* **Materials 14,** (19) 5773 (2021).

38. Synthesis and characterization of SnO_2-doped AZO thermoelectric thin films, *Giovanna Latronico,* ***Saurabh Singh****, Pan Sian Wei, Yukihiro Kawamura, Chihiro Sekine, Takahiro Baba, Takao Mori, Tsunehiro Takeuchi, Ataru Ichinose, Sergey Sarkisov, Simeon Wilson, Abdalla Darwish, and Paolo Mele*, **Materials 14,** (22), 6929 (2021).

39. Magnetic behavior of Ru substituted skyrmion metal MnSi, *S. Shanmukharao Samatham,* ***Saurabh Singh****, Akhilesh Kumar Patel, and K. G. Suresh,* **J. Phys.: Condens. Matter 34,** 345801 (2022).

Research Publications (in Conference Proceedings)

1. Fabrication of a simple apparatus for the Seebeck coefficient measurement in temperature range 300-600 K, ***Saurabh Singh*** *and Sudhir K. Pandey,* **AIP Conference Proceedings 1832**, 060006 (2017).
2. Theoretical study of thermopower behavior of $LaFeO_3$ compound in high temperature region, ***Saurabh Singh***, *Shivprasad S. Shastri, and Sudhir K. Pandey*, **AIP Conference Proceedings**, **1942**, 110018 (2018).
3. Investigation of thermoelectric properties of $LaFe_{0.1}Co_{0.9}O_3$ compound, ***Saurabh Singh***, *Shubham Singh, Ashutosh Patel, and Simant Kumar Srivastav,* **AIP Conference Proceedings**, **2115**, 030614 (2019).
4. Electronic structure and thermoelectric properties of Co_2CrGa using first principles calculations, *Shubham Singh,* ***Saurabh Singh***, *Nitin Kumar Bijewar, and Ashish Kumar*, **AIP Conference Proceedings**, **2115**, 030368 (2019).
5. Investigation of Thermoelectric properties of Magnetic Insulator FeRuTiSi Using First Principle Calculation, ***Saurabh Singh***, *Shubham Singh, Nitinkumar Bijewar, and Ashish Kumar*, **AIP Conference Proceedings 2265**, 030453 (2020).
6. Thermoelectric properties of Half-Metallic FeMnScGa Using First Principle Calculation, *Shubham Singh,* ***Saurabh Singh***, *Nitinkumar Bijewar, and Ashish Kumar*, **AIP Conference Proceedings 2265**, 030649 (2020).

Oral Presentation in conferences/Workshop/Seminar

1. "*Improving the thermoelectric properties of non-toxic and flexible Ag_2S material by electronic structure modification*", **Saurabh Singh***, Keisuke Hirata, Gareoung Kim, Dogyun Byeon, Takashi Nagaya, Omprakash Muthusamy, Masaharu Matsunami, Tsunehiro Takeuchi, **Virtual Conference on Thermoelectrics,** July 21st - 23rd 2020 using the Zoom platform.
2. *"Flexible thermoelectric materials for wearable device applications",* **Shibaura IT Virtual Workshop on Materials for Energy,** organized by Shibaura Institute of Technology, College of Engineering, Tokyo, Japan, **16th July 2020.** (**Invited talk**)
3. *"Development of Simple, Low Cost, and Fully Automated Systems for Seebeck, Resistivity, and Thermal Conductivity Measurement"* **General and Sustainable Chemistry Special Lecture Series on Advanced Materials Science,** organized by Shibaura Institute of Technology, College of Engineering, Tokyo, Japan, **16th July 2020.** (**Invited talk**)
4. *"Design and fabrication of low cost automatic measurement systems for characterization of Thermoelectric materials"*, **THREE DAY INTERNATIONAL WEBINAR ON EMERGING TREND IN MATERIAL SCIENCE-2020 (IWETMS-2020)** Organized by Department of Physics MAHARAJA BHOJ GOVT. PG COLLEGE, DHAR (M.P.), INDIA in association with IAPT RC-09 **05th July-2020.** (**Invited talk**)
5. *"Study of Thermoelectric Properties of Oxide Material in High-Temperature Region"*, **A Faculty Development Programme On NANO SCIENCE AND TECHNOLOGY (ENERGY, ENVIRONMENT AND HEALTHCARE)** organized by Sathyabama Institute of Science and Technology; and Indian Institute of Information Technology, Design and Manufacturing (IIITDM) Kancheepuram, India, **1st July 2020.** (**Invited talk**)

6. *"Development of Non-Toxic and Flexible Ag_2S Based Thermoelectric Material for Energy Applications",* **Saurabh Singh***, Keisuke Hirata, Gareoung Kim, Dogyun Byeon, Omprakash Muthusamy, Masaharu Matsunami, Tsunehiro Takeuchi, **The 81st JSAP Autumn Meeting (JSAP-2020) September 08-11,** Doshisha University, Imadegawa Campus, Kyoto, Japan.
7. "*Importance of e-learning in research after covid 19*" **Motivational talk on future opportunity in field of science and technology after under-graduation** though Skype, to B.Sc. Physics (Third year students), Thakur College of Science and Commerce, Kandivali, Mumbai, Maharashtra India.
8. *"Both p and n-type flexible thermoelectric materials based on Ag_2S by the electronic structure modification",* **Saurabh Singh*** Keisuke Hirata, Dogyun Byeon, Gareoung Kim, Takashi Nagaya, Takuya Matsunaga, Masaharu Matsunami, Tsunehiro Takeuchi, **CREST mini workshop**, December 14-15, 2019 C122, Kurokami-Minami E1, Kumamoto University, Japan.
9. *"Flexible Inorganic Thermoelectric Materials $Ag_2(S_{1-x}Se_x)$"* **Saurabh SINGH***, Keisuke HIRATA, Takuya MATSUNAGA, Dogyun BYEON, Masaharu MATSUNAM, Tsunehiro TAKEUCHI, **Materials Research Meeting 2019 (MRM2019)**, December 10-14, Yokohama, Japan.
10. *"Electronic structure and thermoelectric properties of flexible Ag_2S based materials",* **Saurabh Singh***, Keisuke Hirata, Dogyun Byeon, Takuya Matsunaga, Masaharu Matsunami, Tsunehiro Takeuchi, **CREST mini workshop**, October 26th, 2019, Toyota technological Institute Nagoya, Aichi, Japan.
11. *"Improvement of thermoelectric properties of Ag_2S by Se substitution"*, **Saurabh Singh*,** Keisuke Hirata, Dogyun Byeon, Swapnil Ghodke, Masaharu Matsunami, Masahiro Adachi, Yoshiyuki Yamamoto, Tsunehiro Takeuchi, **The 80th JSAP Autumn Meeting (JSAP-2018),** September 18-21, Hokkaido University, Sapporo Campus, Hokkaido, Japan.
12. *"Investigation of electronic and thermoelectric properties of $Ag_{2-x}TM_xS$ (TM = Ti, V, Cr, Mn, Fe, Co, Ni, Cu) from first principle calculations",* **Saurabh Singh***, K. Hirata, M. Adachi, Y. Yamamoto, M. Matsunami, T. Takeuchi, **The 16th Thermoelectric Society of Japan (TSJ2019)** September 2 - 4, 2019, Nagoya Institute of Technology Gokisho Campus, Nagoya, Japan.
13. *"Thermoelectric Properties of $Ag_2(S_{1-x}Se_x)$"*, **Saurabh Singh***, Keisuke Hirata, Dogyun Byeon, Omprakash Muthusamy, Masaharu Matsunami, Tsunehiro Takeuchi, **The 38th International & 4th Asian Conference on Thermoelectrics (ICT/ACT 2019),** June 30 - July 4, Gyeongju, South Korea.
14. *"Development of Flexible Inorganic Thermoelectric Materials Using $Ag_2(S,Se)$"*, **Saurabh Singh***, Keisuke Hirata , Takuya Matsunaga, Dogyun Byeon, Masaharu Matsunami, Tsunehiro Takeuchi, **CREST mini workshop,** 8-9 June 2018**,** C209 Center building, Okinawa Institute of Science and technology (OIST), Okinawa, Japan
15. *"Thermoelectric Properties of $La_{1-x}Ba_xCoO_3$ (x = 0.18, 0.25, & 0.5) Compound: Experiment and Theory",* **Saurabh Singh*** and Sudhir K Pandey, **National Conference on Recent Trends in Experimental and Theoretical Physics (NCRTETP - 2017),** 23rd - 24th November 2017, Sri Sai University, Palampur, H.P. India.
16. *"Experimental and Theoretical Study of Oxide Materials for Thermoelectric Applications",* **Saurabh Singh*** and Sudhir K Pandey, **Conference on Spectroscopy of Emerging Functional Materials (SEFM 2017),** 9-10 October 2017, Indian Institute of Technology Mandi, Himachal Pradesh-175001, India.
17. "*Experimental and Theoretical tools for the investigation of Thermoelectric Properties"*, **Saurabh Singh*** and Sudhir K Pandey, **School on Characterizations of Materials, 4-9 September 2017**, Inter University Accelerator Center (IUAC), New Delhi, India. (**Invited talk)**
18. *"Investigation of High Temperature Thermoelectric Properties of Oxide Materials",* **Saurabh Singh*** and Sudhir K Pandey, **IUMRS-ICAM 2017, The 15th International Conference on**

Advanced Materials, 27th August - 1st September 2017, Yoshida Campus Kyoto University, Kyoto, Japan.

19. *"High Temperature Thermoelectric Properties of Oxide Materials"*, **Saurabh Singh*** and Sudhir K Pandey, **ANUSANDHAN- 2017**, 04-March, Indian Institute of Technology Mandi, Himachal Pradesh-175001, India. (***Best Oral presentation award)***
20. *"Study of thermoelectric behavior by using various tools"*, **Saurabh Singh*** and Sudhir K Pandey, **Advanced Materials Research Center (AMRC) symposium 2015**, 29-30 May, Indian Institute of Technology Mandi, Himachal Pradesh-175001, India.
21. *"A Fully Automated Precise Measurement System for Ultrasonic Velocity and Attenuation in Solids Down to Liquid Helium Temperatures and Magnetic Field ± 14 Tesla using Pulse Transmission Technique", **Saurabh Singh*** and Alok banerjee,* **National Seminar on Materials Characterization by Ultrasonics"** (NSMCU-2012) 3-4 April 2012, Amity School of Engineering & Technology, Bijwasan, New Delhi. (***Best Oral presentation award)***

Reviewer in Peer Reviewed Journals

Journal of Advanced Ceramics, Journal of American Ceramic Society, Journal of Physics Condensed Matter (**JPCM**), Journal of Physics D Applied Physics, Japanese Journal of Applied Physics (**JJAP**), Physica Scripta, Materials Research express (**MRX**), Applied Physics Letter (**APL**), AIP Advances, Review of Scientific Instruments (**RSI**), Journal of Alloys and Compounds (**JALCOM**), Intermetallic, Superlattices and Microstructures, Vacuum, Physica E: Low-dimensional systems and Nanostructures, The Journal of biological and Chemical Luminescence, International Journal of Energy Research, Advanced in Condensed Matter Physics, Journal of Electronic Materials (**JEM**), Ceramics International, Philosophical Magazine, Applied Physics Express (**APEX**). International Journal of Sensors, Wireless Communications and Control.

Guest Editor in Scientific Journals

- Special Issue **"Emergent Thermoelectric Materials for Energy Applications" Journal:** *Crystals* (ISSN 2073-4352) **[**10 November 2021 - 10 June 2022] https://www.mdpi.com/journal/crystals/special_issues/emergent_thermoelectric

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